Dielectronic recombination for average ions

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Dielectronic recombination (DR) in the average-atom (AA) model has been studied. The reasonableness of directly applying the Burgess-Merts (BM) formula to the AA model has been examined. We have noticed that it is inappropriate to use the BM formula to calculate DR rate coefficients for average ions. We have developed a self-consistent-field theoretical method to treat the DR for average ions with electrons. As an example, the DR rate coefficients for argon have been calculated at a defined electron population, and have been compared with the rate-coefficient average via detailed configuration accounting. [S1050-2947(97)06101-5]

I. INTRODUCTION

The average-atom (AA) model [1–4] is an efficient approximate method in the calculations of radiation transport in high-temperature laser-created plasmas. The numerical simulations using the AA model have successfully reproduced the x-ray conversion efficiency. However, the calculated x-ray spectra do not coincide with the experimental ones [5,6]. The discrepancies were considered to originate in the atomic physics modeling [5–8]. The employed nonlocal-thermodynamic-equilibrium atomic physics model included average-ion semiempirical or hydrogenic rates and neglected subshell splitting. Obviously, it is necessary to improve rate coefficients for various atomic processes. This paper focuses on the study of dielectronic recombination (DR) processes for average ions. First of all, we examine the reasonableness of directly applying the Burgess-Merts (BM) formula [9] to the AA model. The DR rate coefficients for average ions have been derived from the rate equations for detailed configuration accounting. Based on the result obtained, we have noticed that the BM formula widely employed in the AA model [2–4,6,8] is inappropriate to this model. This is because the BM formula can only give the rate coefficients summed over the final states [9–11], whereas the AA model needs the recombination rates in a special state. We have proposed a self-consistent-field theoretical method to treat DR for average ions with electrons. This method includes l splitting and can give the required recombination rates in a special final state. Also we have developed an average-atom structure program. As an example, the rate coefficients for argon have been calculated at a defined electron population, and have been compared with the rate-coefficient averages via detailed configuration accounting.

II. THEORY

With the framework of the AA model, the DR for the ionic species present in the plasmas can be replaced with that for a single fictitious "average ion" [1–3]. The DR rate coefficients for average ions can be derived from the rate equations for detailed configuration accounting. Here, for simplicity we only consider the contribution from DR to the density change of ions. Thus the rate equation for the density $N_{z,n}$ of an ion in the charge state z with an excited- or

ground-state electron in the nth level can be written as [4]

$$\frac{dN_{z,n}}{dt} = -\sum_m \alpha_{z,n;z-1,m} N_{z,n} N_e + \sum_{m'} \alpha_{z+1,m';z,n} N_{z+1,m'} N_e,$$

(1)

where $\alpha_{z,n;z-1,m}(\alpha_{z+1,m';z,n})$ are the DR rate coefficients of an ion $N_{z,n}(N_{z+1,m'})$ in a recombined ion $N_{z-1,m}(N_{z,n})$, and N_e is the free-electron density. The electron energy levels in Eq. (1) are distinguished by the principal and angular momentum quantum numbers $(n_i l_i)$. Let $\xi_{k;z,n}$ denote the number of electrons in the kth levels of a "real ion" $(N_{z,n})$. Multiplying Eq. (1) with $\xi_{k;z,n}$ and summing over different charge states z and levels n, we have

$$\sum_{z,n} \xi_{k;z,n} \frac{dN_{z,n}}{dt} = -\sum_{z,n,m} \xi_{k;z,n} \alpha_{z,n;z-1,m} N_{z,n} N_e$$

$$+ \sum_{z,n,m'} \xi_{k;z,n} \alpha_{z+1,m';z,n} N_{z+1,m'} N_e.$$

(2)

In the second term of the right side of Eq. (2), if one replaces $z+1$ by z, exchanges m' and n, and drops the prime symbol of m', then the results of the summation over z, n, and m' are not affected. Therefore Eq. (2) can be written in the form

$$\frac{d}{dt}\left(\sum_{z,n} \xi_{k;z,n} N_{z,n}\right) = \sum_{z,n,m} (\xi_{k;z-1,m} - \xi_{k;z,n})$$

$$\times \alpha_{z,n;z-1,m} N_{z,n} N_e$$

$$= \sum_{z,m} (\xi_{k;z-1,m} - \xi_{k;z,g}) \alpha_{z,g;z-1,m} N_{z,g} N_e$$

$$+ \sum_{z,m} \sum_{n \neq g} (\xi_{k;z-1,m} - \xi_{k;z,n})$$

$$\times \alpha_{z,n;z-1,m} N_{z,n} N_e,$$

(3)

where according to the different ions $(N_{z,n})$ present in the plasmas, k is either a ground-state (g) or an excited-state level. Hence, for a given k, all these ions can be divided into the $k=g(N^{\mathrm{I}}_{z,n})$ and $k \neq g(N^{\mathrm{II}}_{z,n})$ groups. For example, when

$k=2p$, $N_{1s^22s^22p^5}$, and N_{1s^22p}, respectively, belong to the $N_{z,n}^{\mathrm{I}}$ and $N_{z,n}^{\mathrm{II}}$ ion groups. Thus Eq. (3) can be rewritten as

$$\frac{d}{dt}\left(\sum_{z,n}\xi_{k;z,n}N_{z,n}\right)=\sum_{z,m}(\xi_{k;z-1,m}-\xi_{k;z,g})\alpha_{z,g;z-1,m}$$
$$\times(N_{z,g}^{\mathrm{I}}+N_{z,g}^{\mathrm{II}})N_e$$
$$+\sum_{z,m}\sum_{n\neq g}(\xi_{k;z-1,m}-\xi_{k;z,n})$$
$$\times\alpha_{z,n;z-1,m}(N_{z,n}^{\mathrm{I}}+N_{z,n}^{\mathrm{II}})N_e.\quad(4)$$

We will, respectively, consider the contributions from the $k=g$ and $k\neq g$ ion groups.

(1) For the $N_{z,n}^{\mathrm{I}}$ ion group, $\xi_{k;z-1,m}-\xi_{k;z,g}=0$ since the electron number of the recombining ($N_{z,g}^{\mathrm{I}}$) and recombined ($N_{z-1,m}^{\mathrm{I}}$) ions in the ground level is equal; and $\xi_{k;z-1,m}-\xi_{k;z,n}=1$ or 0 ($n\neq g$), respectively, for the ions whose configurations are of the form $1s^22s^2\cdots(k-1)^{4l_{k-1}+2}k^{0\sim4l_k+1}n$ ($n=k+1,k+2,\ldots$) and for the other ions. Therefore

$$\sum_{z,m}(\xi_{k;z-1,m}-\xi_{k;z,g})\alpha_{z,g;z-1,m}N_{z,g}^{\mathrm{I}}N_e=0,\quad(5)$$

$$\sum_{z,m}\sum_{n\neq g}(\xi_{k;z-1,m}-\xi_{k;z,n})\alpha_{z,n;z-1,m}N_{z,n}^{\mathrm{I}}N_e$$
$$=\sum_{z_k,n\neq g}\left(\sum_m\alpha_{z_k,n;z_k-1,m}\right)N_{z_k,n}^{\mathrm{I}}N_e,\quad(6)$$

where the summation over z in the right side of Eq. (6) has been changed into that over z_k, and z_k represents the charge state, in which the ions are of the $1s^22s^2\cdots(k-1)^{4l_{k-1}+2}k^{0\sim4l_k+1}n$ ($n=k+1,k+2,\ldots$) configuration form. Equation (6) means that the DR for only these ions, whose configurations are of the above form, contributes to the change of electron number in the k level.

(2) For the $N_{z,n}^{\mathrm{II}}$ ion group, the difference between the electron number of the recombining ($N_{z,n}^{\mathrm{II}}$) ions and that of recombined ($N_{z-1,m}^{\mathrm{II}}$) ions in the k level may be expressed in terms of the Kronecker symbols. $\xi_{k;z-1,m}-\xi_{k;z,g}=\delta_{km}$ and $\xi_{k;z-1,m}-\xi_{k;z,n}=\delta_{km}-\delta_{kn}$. This is because the DR makes only the m level increase an electron for the $N_{z,g}^{\mathrm{II}}$ ions, and the change of electron number happen only in the m and n levels for the $N_{z,n}^{\mathrm{II}}$ ($n\neq g$) ions. Thus we get

$$\sum_{z,m}(\xi_{k;z-1,m}-\xi_{k;z,g})\alpha_{z,g;z-1,m}N_{z,g}^{\mathrm{II}}N_e$$
$$=\sum_z\alpha_{z,g;z-1,k}N_{z,g}^{\mathrm{II}}N_e,\quad(7)$$

$$\sum_{z,m}\sum_{n\neq g}(\xi_{k;z-1,m}-\xi_{k;z,n})\alpha_{z,n;z-1,m}N_{z,n}^{\mathrm{II}}N_e$$
$$=\sum_{\substack{z,n\\n\neq g}}\alpha_{z,n;z-1,k}N_{z,n}^{\mathrm{II}}N_e-\sum_{\substack{z,m\\k\neq g}}\alpha_{z,k;z-1,m}N_{z,k}^{\mathrm{II}}N_e.\quad(8)$$

Substituting Eqs. (5)–(8) into Eq. (4), and merging Eq. (7) and the first term of Eq. (8) into a term, we finally obtain

$$\frac{d}{dt}\left(\sum_{z,n}\xi_{k;z,n}N_{z,n}\right)=\sum_{z,n}\alpha_{z,n;z-1,k}N_{z,n}N_e$$
$$-\sum_{\substack{z,m\\k\neq g}}\alpha_{z,k;z-1,m}N_{z,k}^{\mathrm{II}}N_e$$
$$+\sum_{z_k,n\neq g}\left(\sum_m\alpha_{z_k,n;z_k-1,m}\right)N_{z_k,n}^{\mathrm{I}}N_e,$$
$$(9)$$

where the superscript II of $N_{z,n}^{\mathrm{II}}$ in the first term of Eq. (9) is dropped. The reason for doing so is that $\alpha_{z,n;z-1,k}=0$ for the $N_{z,n}^{\mathrm{I}}$ ion, so to add $\sum_{z,n}\alpha_{z,n;z-1,k}N_{z,n}^{\mathrm{I}}N_e$ to the first term obviously does not affect the results of this term. In addition, the latter two terms in the equation are the contributions from the partial ions in the excited states, hence can be neglected [12]. Concerning this, a detailed discussion will be given in Sec. III. Thus Eq. (9) reduces to

$$\frac{d}{dt}\left(\sum_{z,n}\xi_{k;z,n}N_{z,n}\right)=\sum_{z,n}\alpha_{z,n;z-1,k}N_{z,n}N_e.\quad(10)$$

In general, in high-temperature laser-created plasmas the distribution of z sharply peaks at $z=z^a$, so one may assume that $\alpha_{z,n;z-1,k}$ for the neighboring ions can be approximated by $\alpha_{z^a,k}$ for an average ion, namely,

$$\alpha_{z^a,k}=\frac{1}{N}\sum_{z,n}\alpha_{z,n;z-1,k}N_{z,n}.\quad(11)$$

By inserting Eq. (11) into Eq. (10) and defining $c_kp_k=(1/N)\sum_{z,n}\xi_{k;z,n}N_{z,n}$, we arrive at

$$\frac{d}{dt}(Nc_kp_k)=N_eN\alpha_k^{dr},\quad(12)$$

where c_kp_k is the occupation number in the k level of average ions, and $\alpha_k^{dr}\equiv\alpha_{z^a,k}$ is the DR rate coefficient in the k level for average ions. From Eqs. (10)–(12), it may be clearly seen that the AA model needs the DR rate coefficients in a special state. In order to make it practical to evaluate the DR rates for average ions with noninteger occupation numbers, we propose that α_k^{dr} be expressed in terms of the configuration-average dielectronic capture rate [13,14]. Let m indicate an initial level, and $j\bar{j}$ be a doubly excited level in DR processes, then α_k^{dr} is

$$\alpha_k^{dr} = \sum_{\substack{m(<k)j(>m) \\ (\bar{j}=k,\ \bar{j}\neq j)}} c_m p_m (1-p_j)(1-p_{\bar{j}}) \beta_{mj\bar{j}}^{(0)} B_{j\bar{j}\rightarrow mk}$$

$$+ \sum_{\substack{m(<k) \\ (j=\bar{j}=k>m)}} c_m p_m (1-p_j)\left(1 - \frac{c_j}{c_j-1}p_j\right)$$

$$\times \beta_{mj\bar{j}}^{(0)} B_{j\bar{j}\rightarrow mk}, \qquad (13)$$

where c_i and p_i ($i = m$, j, and $\bar{j}$), respectively, are the statistical weight and the electron occupation probability of the i

subshell; $\beta_{mj\bar{j}}^{(0)}$ is the dielectronic capture coefficient for a hypothetical one-electron ion, defined by

$$\beta_{mj\bar{j}}^{(0)} = \frac{h^3}{(2\pi m_e k_B T)^{3/2}} \frac{g_{j\bar{j}}}{g_c g_m} A_{j\bar{j}m}^a e^{-\epsilon_c/k_B T} \qquad (14)$$

and $B_{j\bar{j}\rightarrow mk}$ is the branching ratio. In terms of the configuration-average Auger and radiative rates, $B_{j\bar{j}\rightarrow mk}$ can be written as

$$B_{j\bar{j}\rightarrow mk} = \frac{c_j p_j'(1-p_m')A_{jm}^r}{c_j p_j' c_{\bar{j}} p_{\bar{j}}'(1-p_m')A_{j\bar{j}m}^a + c_j p_j'(1-p_m')A_{jm}^r + c_{\bar{j}} p_{\bar{j}}'(1-p_m')A_{\bar{j}m}^r} \qquad (j\neq\bar{j}), \qquad (15)$$

$$B_{j\bar{j}\rightarrow mk} = \frac{c_j p_j'(1-p_m')A_{jm}^r}{\frac{1}{2}c_j p_j'(c_j p_j' - 1)(1-p_m')A_{j\bar{j}m}^a + c_j p_j'(1-p_m')A_{jm}^r} \qquad (j=\bar{j}). \qquad (16)$$

In Eqs. (14)–(16), the statistical weight factor term $g_{j\bar{j}}/g_c g_m$ is equal to $c_j c_{\bar{j}}/2c_m$ for $j\neq\bar{j}$, and $c_j(c_j-1)/4c_m$ for $j=\bar{j}$, respectively. $A_{j\bar{j}m}^a$ is the Auger rate for a hypothetical two-electron ion [13,14]. A_{jm}^r is the radiative decay rate for a hypothetical one-electron ion [13]. $p_j' = p_j + \delta$, here $c_j\delta$ is the number of excited electrons, and less than or equal to one. When $j\neq\bar{j}$, for $\min(c_m p_m, c_j - c_j p_j, c_{\bar{j}} - c_{\bar{j}} p_{\bar{j}}) \geq 1$ and <1, we choose $\delta = 1/c_j$ and $\delta = \min(c_m p_m, c_j - c_j p_j, c_{\bar{j}} - c_{\bar{j}} p_{\bar{j}})/c_j$, respectively. When $j=\bar{j}$, we choose $\delta = 2\min(c_m p_m, (c_j - c_j p_j)/2)/c_j$ for $c_m p_m < 1$, $\delta = 2/c_j$ for $c_m p_m \geq 1$ and $c_j p_j \leq c_j - 2$, and $\delta = 1-p_j$ for $c_m p_m \geq 1$ and $c_j - 2 < c_j p_j < c_j - 1$. It should be pointed out that Eqs. (13), (15), and (16) are independent of the particular coupling scheme. Furthermore, we emphasize that Eqs. (15) and (16) omit radiative transitions to non-m subshells. This is because the resonance transitions j or $\bar{j}\rightarrow m$ are normally much faster than the other transitions [15].

III. RESULTS AND DISCUSSION

An atom-structure program has been developed in the AA model, in which the occupation number of orbital electrons is a noninteger in general. The Hartree-Fock equations are solved self-consistently to obtain the radial wave functions $P_{nl}(r)$ and the orbital energies ε_i. Here for the orbital with an occupation number less than one, the direct and exchange self-interaction terms in the central potential are multiplied by a factor which is just the occupation number to just cancel out the self-energy involved in both the direct and exchange sum. The continuum orbital wave function $P_{l_c}(r)$ required in computing the Auger matrix elements is obtained in the distorted-wave approximation, and normalized per unit Rydberg. The energy of free electrons in Eq. (14) is fixed by the

difference of the orbital energies: $\varepsilon_c = \varepsilon_j + \varepsilon_{\bar{j}} - \varepsilon_m$. As an example, we have calculated the DR rate coefficients for argon in the $3s$ and $3p$ subshells at the bound electron populations: $c_{1s}p_{1s}=2.0$, $c_{2s}p_{2s}=2.0$, $c_{2p}p_{2p}=3.999$, $c_{3s}p_{3s}=0.05$, $c_{3p}p_{3p}=0.025$. The results calculated at several temperature points are listed in Table I. It should be pointed out that we have made two approximations to obtain DR rates for average ions in the AA model. First, the DR from the partial excited states has been neglected. The reason this is a good approximation follows. At the electron density $N_e < 10^{22}$ cm^{-3}, the excited-state level populations are usually much less than the ground-state populations, but the total DR rate coefficients from the two kinds of states are approximately equal. Therefore the total DR rates from the excited states are much smaller than the total DR rates from the ground states, and can be neglected in the calculation [12]. Second, the DR rate coefficients for the various ions present in high-temperature plasmas have been approximated by that for a single fictitious ''average ion.'' This approximation originates in a basic assumption in the AA model

TABLE I. DR rate coefficients for the average Ar ion in the $3s$ and $3p$ subshells in units of cm^3/sec. Numbers in square brackets are powers of 10.

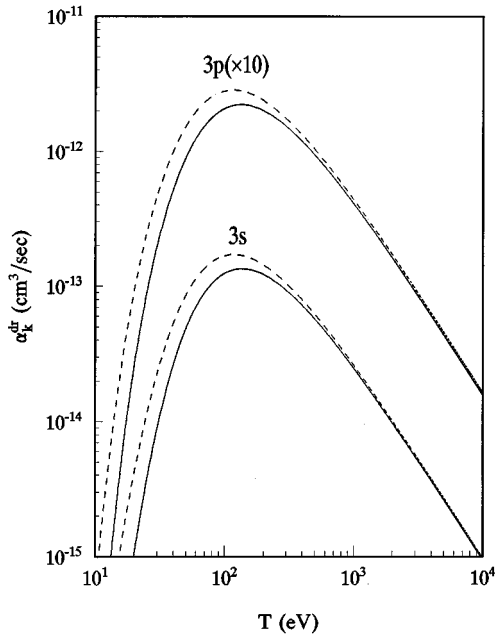| T (keV)	α_{3s}^{dr}	α_{3p}^{dr}
0.1	1.247[−13]	2.085[−13]
0.3	9.357[−14]	1.538[−13]
0.5	5.725[−14]	9.427[−14]
1.0	2.489[−14]	4.109[−14]
3.0	5.500[−15]	9.100[−15]
5.0	2.628[−15]	4.350[−15]
10.0	9.486[−16]	1.571[−15]

FIG. 1. DR rate coefficients for average Ar ion in the $3s$ and $3p$ subshells vs electron temperature. The solid curve shows the rate coefficients for the average ion, while the dashed curve shows the rate-coefficient averages via detailed configuration accounting. The DR rate coefficients in the $3p$ subshell are multiplied by 10.

FIG. 2. DR rate coefficients for the ''real'' Se^{24+} ion in the $3s$, $3p$, and $3d$ subshells vs electron temperature. The solid curve and the dashed curve indicate the results of this calculation and Hagelstain's, respectively. The DR rate coefficients in the $3d$ subshell are multiplied by 10.

[1–3]. Namely, an average ion represents a close approximation to the canonical average. However, there is very little detailed analysis of this problem. Generally, it is believed that for heavier ions it is reasonable to assume that the two averages are close, and for lighter ions the difference may be significant. Rozsnyai [16] has compared the energy of the average ion and the energy average via detailed configuration accounting for helium at $T=5$ eV. The results have shown that the difference between the two methods was about 20%. Here, we have numerically made an examination of the rate coefficients for the average Ar ion at the bound electron population given above. First of all, for the given average population p_i and statistical weight c_i, we have employed a statistical method, as made by Takabe and Nishikawa [8], to obtain the fractional distribution $N_{z,n}/N$ of each electronic configuration. Then the DR rate coefficients for each configuration have been explicitly calculated by using the self-consistent method [17,18]. Finally, we have evaluated the rate-coefficient average. The rate coefficients for the average ion and the rate-coefficient averages via detailed configuration accounting have been compared in Fig. 1. Comparisons show that for recombination into the two subshells, the difference is smaller than a factor of one at $T \geqslant 40$ eV, but increases with decreasing T. The greater difference in the range of lower temperature can be traced to the AA model. The DR rate coefficient for average ions includes an exponential factor $e^{-\varepsilon_c/T}$, in which the determination of ε_c is related to average ions. At low temperature, a little ε_c error may give rise to a large α_k^{dr} difference.

More, Zimmerman, and Zinamon [15] have formulated a method to add DR to the AA model, and the strong correlations of electron populations induced by the dielectronic capt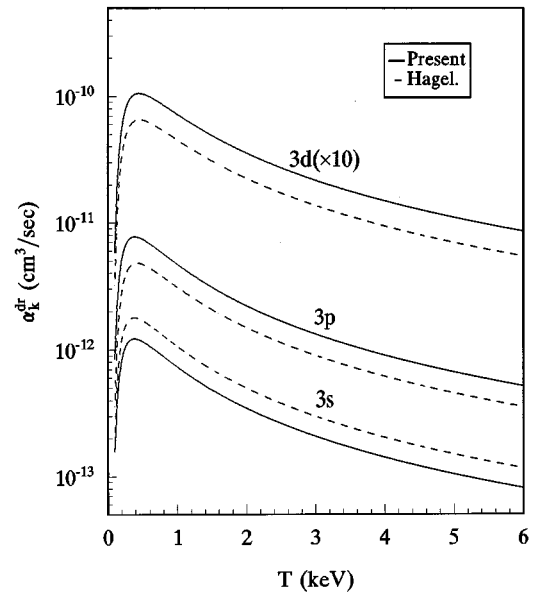ure process have been studied. But the DR rate coefficients have not been explicitly evaluated in Ref. [15]. So any comparison cannot be made with the work of More, Zimmerman, and Zinamon. In order to test the present method, we have calculated the DR rate coefficients for the ''real'' Se^{24+} ion by using our code in the AA model, and compared our results with Hagelstain's [19] in Fig. 2. In our calculations, the doubly excited states included are the $3l3l'$ intermediate autoionization states, corresponding to that in Ref. [19], and only the transitions where the excited electron can return to its original subshell by spontaneous radiation are taken into account. From Fig. 2, we may see that the difference between the elaborate calculations and our results is less than a factor of 1. In view of the fact that we adopt the extremely simple form to calculate the Auger and radiative rates, the existence of the above error is obvious.

IV. SUMMARY AND CONCLUSIONS

In conclusion, from Eqs. (10)–(12), it may be clearly seen that the AA model needs the DR rate coefficients in a special state, not the ones summed over the final states. Therefore the Burgess-Merts formula cannot be directly applied to the AA model. We have proposed a self-consistent-field theoretical method to calculate DR rates for average ions, and also developed an average-atom structure program to calculate the required recombination rate coefficients in a special state in the AA model. As an example, the DR rate coefficients for argon have been calculated at a defined electron population, and have been compared with the rate-coefficient average via detailed configuration accounting. To test the present method, we have evaluated the DR rate coefficients for the ''real'' Se^{24+} ion using our code in the AA model. Comparisons with the other elaborately calculated results

have illustrated the reasonableness of the present method. It is very interesting to calculate the x-ray spectra or other quantities by adopting the DR rate coefficients from the present method, and then observe the improvements resulted. Hence it is worth investigating further. However, this involves a great deal of complicated work. We plan to discuss this problem in future work.

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